



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:06 AM UTC

PDB ID : 4YY0 / pdb_00004yy0
Title : The structure of hemagglutinin from a H6N1 influenza virus (A/chicken/Taiwan/A2837/2013)
Authors : Wang, F.; Qi, J.; Bi, Y.; Zhang, W.; Wang, M.; Wang, M.; Liu, J.; Yan, J.; Shi, Y.; Gao, G.F.
Deposited on : 2015-03-23
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

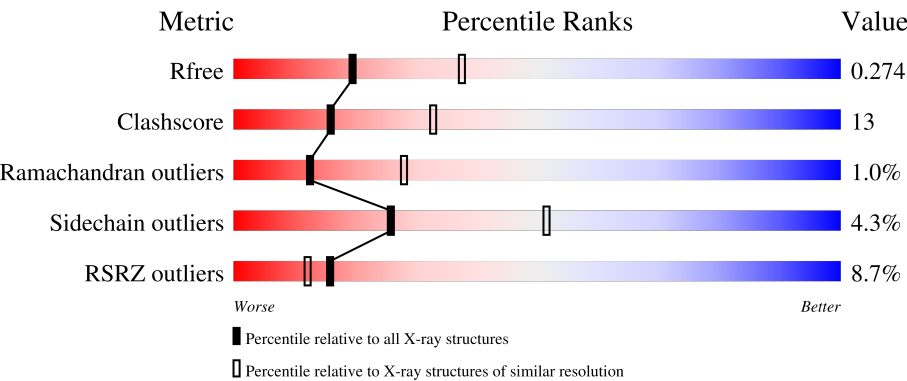
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	4% 83% 14% ..
1	C	325	4% 82% 16% .
1	E	325	8% 77% 20% ..
2	B	159	18% 69% 23% 7% .
2	D	159	14% 63% 31% 5% ..

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Mol	Chain	Length	Quality of chain
2	F	159	15% 62% 27% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11681 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

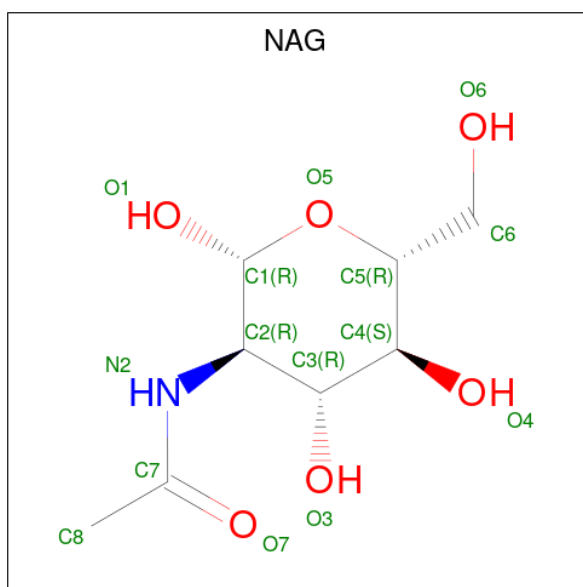
- Molecule 1 is a protein called HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			
1	C	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			
1	E	325	Total	C	N	O	S	0	0	0
			2563	1625	436	489	13			

- Molecule 2 is a protein called HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			
2	D	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			
2	F	159	Total	C	N	O	S	0	0	0
			1275	794	221	253	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	1	Total	O	0	0
			1	1		
4	C	15	Total	O	0	0
			15	15		
4	D	5	Total	O	0	0
			5	5		
4	E	13	Total	O	0	0
			13	13		

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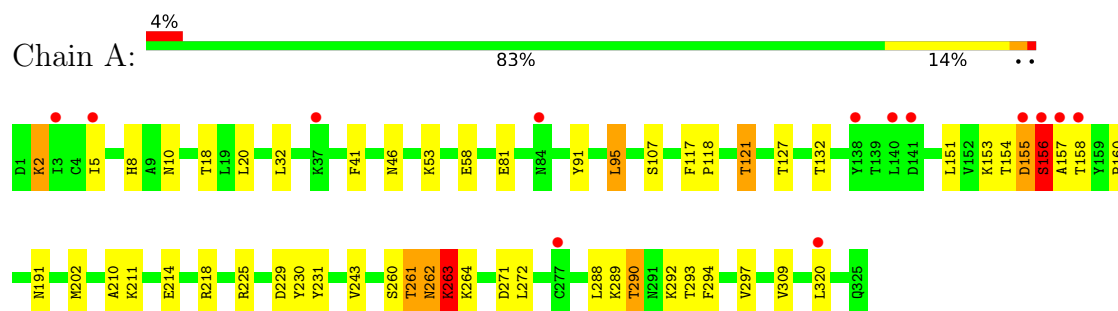
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	5	Total	O	0	0
			5	5		

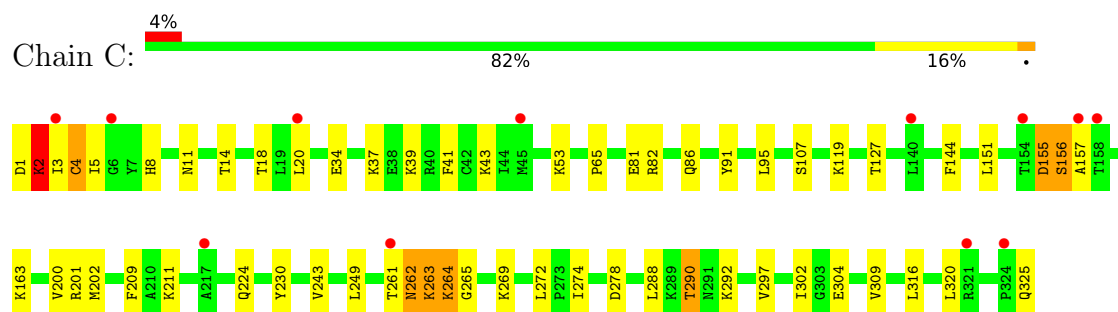
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

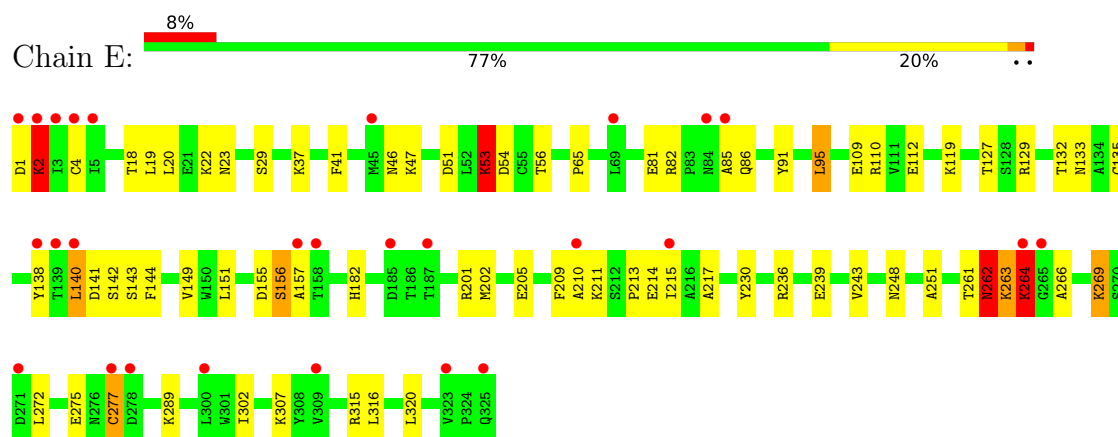
• Molecule 1: HA1



• Molecule 1: HA1

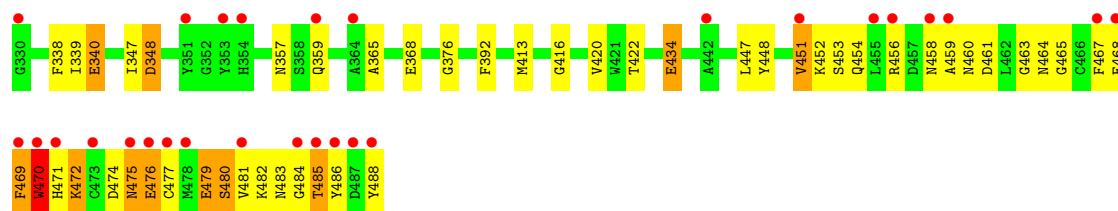


• Molecule 1: HA1



• Molecule 2: HA2

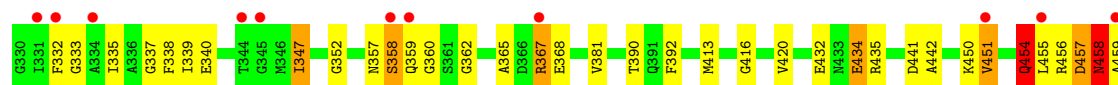




● Molecule 2: HA2



● Molecule 2: HA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.61Å 106.26Å 125.28Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	41.37 – 2.59 41.37 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.37-2.59) 99.2 (41.37-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.220 , 0.271 0.224 , 0.274	Depositor DCC
R_{free} test set	2711 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11681	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/2625	0.92	8/3571 (0.2%)
1	C	0.38	0/2625	0.84	5/3571 (0.1%)
1	E	0.43	0/2625	0.90	9/3571 (0.3%)
2	B	0.57	0/1301	1.22	13/1754 (0.7%)
2	D	0.58	0/1301	1.18	11/1754 (0.6%)
2	F	0.59	1/1301 (0.1%)	1.23	17/1754 (1.0%)
All	All	0.47	1/11778 (0.0%)	1.00	63/15975 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	469	PHE	CG-CD1	-5.11	1.28	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	THR	N-CA-C	-17.92	79.31	109.24
1	E	262	ASN	N-CA-CB	-12.84	88.49	110.32
1	A	262	ASN	N-CA-CB	-11.25	92.98	110.30
2	D	471	HIS	N-CA-C	-9.77	95.79	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	GLY	N-CA-C	-9.53	94.77	112.10
1	E	263	LYS	N-CA-C	8.84	122.55	110.35
2	B	485	THR	CA-C-N	-8.67	109.72	122.65
2	B	485	THR	C-N-CA	-8.67	109.72	122.65
2	D	347	ILE	N-CA-C	-8.63	103.97	112.17
2	D	372	LYS	N-CA-C	-8.53	102.07	111.36
2	D	472	LYS	N-CA-C	8.36	122.70	109.50
2	B	469	PHE	N-CA-C	8.30	122.76	110.48
2	B	475	ASN	N-CA-C	8.15	123.52	113.50
2	F	454	GLN	N-CA-C	-7.96	101.38	112.45
2	D	463	GLY	N-CA-C	-7.93	105.25	114.69
1	A	261	THR	CB-CA-C	-7.85	93.81	109.35
1	E	138	TYR	N-CA-C	-7.69	103.20	112.59
2	F	468	GLU	N-CA-C	7.69	123.14	107.69
2	B	463	GLY	N-CA-C	-7.49	104.93	114.37
2	F	458	ASN	N-CA-C	-7.08	104.51	113.01
2	B	465	GLY	N-CA-C	-6.91	105.56	115.64
2	F	460	ASN	N-CA-C	-6.78	100.19	109.95
2	B	476	GLU	N-CA-C	-6.56	104.91	113.17
2	D	371	GLN	CA-CB-CG	6.51	127.12	114.10
2	F	360	GLY	N-CA-C	6.50	118.71	110.38
2	B	485	THR	N-CA-C	6.43	120.50	111.30
2	F	347	ILE	N-CA-C	6.38	120.38	113.43
2	B	477	CYS	N-CA-C	-6.14	104.66	111.36
2	F	476	GLU	N-CA-C	-6.14	105.75	113.18
2	F	359	GLN	N-CA-C	-6.07	104.77	111.82
2	D	485	THR	CA-C-N	-5.97	115.08	122.84
2	D	485	THR	C-N-CA	-5.97	115.08	122.84
2	F	469	PHE	N-CA-CB	-5.92	101.13	110.06
1	E	53	LYS	CB-CA-C	-5.84	109.29	117.23
1	E	82	ARG	CA-C-N	5.82	126.22	119.47
1	E	82	ARG	C-N-CA	5.82	126.22	119.47
2	F	485	THR	CA-C-N	-5.82	113.10	121.42
2	F	485	THR	C-N-CA	-5.82	113.10	121.42
2	B	470	TRP	N-CA-CB	-5.74	100.80	110.49
2	D	370	THR	CA-C-N	-5.66	113.60	122.65
2	D	370	THR	C-N-CA	-5.66	113.60	122.65
1	E	262	ASN	N-CA-C	-5.59	105.56	112.38
2	F	462	LEU	CA-CB-CG	5.58	135.81	116.30
2	F	362	GLY	N-CA-C	5.53	118.50	111.37
2	F	457	ASP	N-CA-C	-5.46	106.48	114.39
2	B	472	LYS	N-CA-C	-5.45	100.35	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ARG	CA-C-N	5.37	125.44	119.32
1	C	82	ARG	C-N-CA	5.37	125.44	119.32
2	B	460	ASN	CA-C-N	5.34	128.93	121.02
2	B	460	ASN	C-N-CA	5.34	128.93	121.02
2	F	468	GLU	CB-CA-C	-5.32	102.29	111.23
1	A	263	LYS	CA-CB-CG	5.32	124.74	114.10
1	E	4	CYS	N-CA-C	5.27	117.69	109.52
2	F	357	ASN	N-CA-C	-5.27	99.58	110.80
2	F	485	THR	CB-CA-C	-5.22	103.88	111.14
1	A	2	LYS	N-CA-C	5.21	116.73	108.96
1	E	23	ASN	N-CA-CB	-5.19	103.54	111.74
2	D	465	GLY	N-CA-C	-5.11	107.22	115.08
1	C	2	LYS	N-CA-CB	-5.11	103.80	111.56
1	C	4	CYS	N-CA-C	5.10	117.89	109.72
1	A	46	ASN	CB-CA-C	5.03	119.56	111.66
1	A	260	SER	CA-C-N	-5.03	114.58	122.73
1	A	260	SER	C-N-CA	-5.03	114.58	122.73

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	TRP	Peptide
2	B	479	GLU	Peptide
2	F	358	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2563	0	2508	42	0
1	C	2563	0	2508	54	0
1	E	2563	0	2507	74	0
2	B	1275	0	1180	53	0
2	D	1275	0	1178	60	0
2	F	1275	0	1180	58	0
3	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	26	1	0
3	D	14	0	13	3	0
3	E	28	0	26	0	0
4	A	30	0	0	4	0
4	B	1	0	0	0	0
4	C	15	0	0	2	0
4	D	5	0	0	0	0
4	E	13	0	0	3	0
4	F	5	0	0	0	0
All	All	11681	0	11152	300	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:GLU:HB2	1:E:261:THR:CG2	1.86	1.04
1:A:261:THR:CG2	1:A:261:THR:O	2.03	1.02
1:A:261:THR:O	1:A:261:THR:HG22	1.63	0.96
2:B:471:HIS:HD2	2:B:472:LYS:H	1.11	0.94
1:C:2:LYS:NZ	1:C:4:CYS:SG	2.41	0.93
2:B:452:LYS:HG2	2:B:456:ARG:HE	1.33	0.91
2:D:379:ASN:ND2	1:E:19:LEU:O	2.07	0.87
1:C:11:ASN:ND2	4:C:501:HOH:O	2.08	0.86
2:F:474:ASP:OD1	2:F:477:CYS:N	2.08	0.86
2:B:471:HIS:CD2	2:B:472:LYS:H	1.94	0.85
1:A:154:THR:C	1:A:156:SER:H	1.86	0.83
1:C:20:LEU:N	2:D:434:GLU:OE2	2.12	0.83
1:C:325:GLN:NE2	2:D:342:GLY:O	2.11	0.83
2:D:458:ASN:ND2	2:D:486:TYR:OH	2.13	0.82
1:E:109:GLU:HB2	1:E:261:THR:HG22	1.58	0.82
1:E:205:GLU:OE1	4:E:501:HOH:O	1.97	0.82
1:C:263:LYS:O	1:C:264:LYS:CG	2.28	0.81
1:A:107:SER:OG	4:A:501:HOH:O	1.99	0.81
1:E:264:LYS:HB2	1:E:302:ILE:HD11	1.63	0.80
2:B:357:ASN:ND2	2:B:359:GLN:OE1	2.14	0.80
1:E:109:GLU:HB2	1:E:261:THR:HG21	1.63	0.79
2:D:460:ASN:HB2	2:D:470:TRP:CZ2	2.18	0.79
2:D:359:GLN:OE1	2:D:475:ASN:ND2	2.16	0.79
2:B:482:LYS:HD2	2:B:482:LYS:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:456:ARG:NH2	2:F:461:ASP:O	2.18	0.77
2:B:454:GLN:HE22	2:B:484:GLY:C	1.93	0.76
1:C:290:THR:HG23	1:C:292:LYS:H	1.50	0.75
2:B:357:ASN:ND2	2:B:475:ASN:OD1	2.20	0.75
1:C:261:THR:HG23	1:C:263:LYS:H	1.52	0.73
2:F:462:LEU:HD13	2:F:466:CYS:HB2	1.70	0.73
2:F:468:GLU:OE1	2:F:468:GLU:N	2.22	0.73
2:D:458:ASN:HB3	2:D:471:HIS:CE1	2.23	0.73
1:E:261:THR:HB	1:E:263:LYS:HD3	1.70	0.72
2:B:454:GLN:NE2	2:B:484:GLY:O	2.22	0.72
1:C:263:LYS:O	1:C:264:LYS:HG3	1.89	0.71
2:B:348:ASP:OD1	2:B:348:ASP:N	2.24	0.71
1:E:264:LYS:H	1:E:264:LYS:HD2	1.54	0.70
2:F:469:PHE:CE1	2:F:473:CYS:HB2	2.26	0.70
1:C:18:THR:HB	2:D:434:GLU:CG	2.22	0.69
1:E:217:ALA:O	4:E:502:HOH:O	2.09	0.69
1:C:18:THR:HB	2:D:434:GLU:HG2	1.74	0.69
1:E:109:GLU:CB	1:E:261:THR:CG2	2.69	0.69
1:A:154:THR:C	1:A:156:SER:N	2.51	0.68
1:A:18:THR:HB	2:B:434:GLU:HG3	1.74	0.68
2:F:477:CYS:O	2:F:480:SER:HB2	1.93	0.68
1:A:117:PHE:O	4:A:502:HOH:O	2.10	0.67
1:C:263:LYS:O	1:C:264:LYS:HG2	1.94	0.67
2:D:453:SER:O	2:D:456:ARG:NH1	2.27	0.67
2:B:452:LYS:O	2:B:456:ARG:HG2	1.94	0.67
1:E:2:LYS:HD3	2:F:469:PHE:HD2	1.60	0.67
2:B:471:HIS:CD2	2:B:472:LYS:N	2.62	0.67
2:D:356:GLU:HG3	2:D:361:SER:HB2	1.77	0.66
1:E:1:ASP:N	4:E:504:HOH:O	2.26	0.66
2:F:392:PHE:HZ	2:F:413:MET:HE3	1.60	0.66
2:B:470:TRP:CG	2:B:471:HIS:HB2	2.31	0.65
1:E:109:GLU:CB	1:E:261:THR:HG22	2.25	0.65
1:A:261:THR:O	1:A:261:THR:HG23	1.90	0.65
1:E:29:SER:OG	1:E:315:ARG:NE	2.30	0.65
1:C:316:LEU:HD23	2:D:381:VAL:HG22	1.79	0.65
1:E:129:ARG:O	1:E:129:ARG:HG2	1.97	0.65
2:F:460:ASN:ND2	2:F:461:ASP:H	1.94	0.64
2:F:475:ASN:O	2:F:479:GLU:HG2	1.98	0.64
1:A:262:ASN:OD1	1:A:263:LYS:N	2.30	0.64
1:A:210:ALA:O	1:A:211:LYS:HG2	1.98	0.64
1:E:209:PHE:CZ	1:E:211:LYS:HG3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG22	1:A:151:LEU:HD22	1.80	0.63
2:B:471:HIS:HD2	2:B:472:LYS:N	1.91	0.63
2:D:475:ASN:HA	2:D:478:MET:HB2	1.81	0.63
1:E:275:GLU:HB2	1:E:277:CYS:SG	2.39	0.63
1:C:290:THR:CG2	1:C:292:LYS:H	2.12	0.62
1:E:20:LEU:HG	2:F:434:GLU:OE2	1.99	0.62
1:C:3:ILE:CD1	2:D:481:VAL:HG21	2.28	0.62
1:A:156:SER:OG	1:A:157:ALA:N	2.25	0.62
2:F:462:LEU:N	2:F:468:GLU:OE2	2.32	0.62
2:B:470:TRP:CD1	2:B:471:HIS:HB2	2.35	0.62
2:B:482:LYS:HD2	2:B:482:LYS:C	2.24	0.62
1:E:263:LYS:HB3	1:E:264:LYS:HG2	1.81	0.62
1:E:127:THR:HG22	1:E:151:LEU:HD22	1.83	0.61
2:D:352:GLY:HA3	2:D:365:ALA:HA	1.81	0.61
1:E:262:ASN:N	1:E:263:LYS:HD2	2.15	0.61
1:E:140:LEU:CD1	1:E:143:SER:HB2	2.31	0.60
1:E:263:LYS:HD2	1:E:263:LYS:H	1.65	0.60
1:E:54:ASP:OD1	1:E:86:GLN:N	2.32	0.60
1:C:262:ASN:O	1:C:263:LYS:HG2	2.01	0.60
1:A:153:LYS:NZ	1:A:191:ASN:O	2.35	0.59
1:E:266:ALA:HB2	1:E:302:ILE:HD13	1.84	0.59
2:D:359:GLN:HE22	2:D:474:ASP:HA	1.67	0.59
1:A:20:LEU:HG	2:B:434:GLU:OE2	2.02	0.59
2:B:480:SER:OG	2:B:481:VAL:N	2.35	0.59
1:C:261:THR:HG23	1:C:263:LYS:N	2.18	0.59
1:C:264:LYS:O	1:C:302:ILE:HD11	2.02	0.58
2:F:474:ASP:OD1	2:F:476:GLU:N	2.36	0.58
2:B:452:LYS:HB3	2:B:456:ARG:HH21	1.67	0.58
1:C:156:SER:OG	1:C:157:ALA:N	2.37	0.58
1:E:316:LEU:HD23	2:F:381:VAL:HG22	1.86	0.58
2:B:392:PHE:HZ	2:B:413:MET:HE3	1.69	0.57
1:E:110:ARG:NH2	1:E:112:GLU:OE2	2.37	0.57
2:F:460:ASN:HB3	2:F:468:GLU:HB2	1.85	0.57
1:A:154:THR:O	1:A:156:SER:N	2.33	0.57
1:E:51:ASP:HB3	1:E:53:LYS:HE3	1.86	0.57
2:D:483:ASN:OD1	3:D:501:NAG:C7	2.52	0.57
2:D:357:ASN:ND2	2:D:473:CYS:O	2.32	0.57
1:E:262:ASN:HD22	1:E:263:LYS:HE3	1.70	0.57
1:E:129:ARG:NH2	1:E:155:ASP:OD2	2.35	0.57
2:F:479:GLU:O	2:F:483:ASN:HB3	2.05	0.57
2:F:460:ASN:HB2	2:F:470:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LYS:HE3	1:C:39:LYS:HE2	1.86	0.56
1:C:201:ARG:HD3	1:E:215:ILE:O	2.04	0.56
2:F:462:LEU:HD13	2:F:466:CYS:CB	2.35	0.56
1:C:2:LYS:NZ	2:D:466:CYS:SG	2.71	0.56
1:E:129:ARG:HH12	1:E:155:ASP:CG	2.13	0.56
2:F:469:PHE:HB2	2:F:471:HIS:CE1	2.40	0.56
2:B:357:ASN:HD21	2:B:359:GLN:HB2	1.70	0.56
1:C:5:ILE:HD11	2:D:451:VAL:HG21	1.88	0.56
1:E:140:LEU:HD11	1:E:143:SER:HB2	1.88	0.55
2:B:476:GLU:O	2:B:480:SER:HB3	2.05	0.55
1:A:262:ASN:OD1	1:A:262:ASN:N	2.40	0.55
2:B:470:TRP:CD2	2:B:471:HIS:HB2	2.42	0.55
1:C:3:ILE:HD12	2:D:481:VAL:HG21	1.88	0.55
1:E:2:LYS:CD	2:F:469:PHE:HD2	2.20	0.55
2:D:371:GLN:HA	2:D:374:ILE:HB	1.88	0.54
2:F:456:ARG:O	2:F:456:ARG:HG3	2.05	0.54
2:B:459:ALA:HB2	2:B:469:PHE:HA	1.90	0.54
2:F:458:ASN:O	2:F:469:PHE:HA	2.08	0.54
2:F:483:ASN:OD1	2:F:483:ASN:C	2.50	0.54
1:A:229:ASP:HB3	1:A:231:TYR:CE2	2.43	0.54
2:D:485:THR:CG2	3:D:501:NAG:H82	2.37	0.54
2:B:447:LEU:O	2:B:451:VAL:HG12	2.07	0.54
1:A:211:LYS:NZ	1:A:231:TYR:OH	2.33	0.54
2:B:471:HIS:CD2	2:B:472:LYS:O	2.61	0.53
2:F:337:GLY:O	2:F:340:GLU:HG2	2.08	0.53
1:A:2:LYS:HB3	2:B:468:GLU:OE1	2.09	0.53
1:A:263:LYS:HG2	1:A:264:LYS:O	2.09	0.52
2:D:370:THR:O	2:D:373:ALA:HB3	2.10	0.52
1:C:95:LEU:HA	1:C:230:TYR:HB2	1.91	0.52
2:B:448:TYR:O	2:B:452:LYS:HB2	2.10	0.52
1:A:118:PRO:O	1:A:121:THR:OG1	2.21	0.52
2:D:359:GLN:CD	2:D:359:GLN:H	2.16	0.52
1:A:158:THR:O	1:A:160:PRO:HD3	2.09	0.51
1:C:43:LYS:HE3	1:C:278:ASP:OD1	2.10	0.51
1:E:140:LEU:HD13	1:E:142:SER:O	2.11	0.51
2:F:352:GLY:HA3	2:F:365:ALA:HA	1.92	0.51
2:B:459:ALA:CB	2:B:469:PHE:HA	2.40	0.51
2:D:454:GLN:O	2:D:488:TYR:HE2	1.93	0.51
2:F:457:ASP:C	2:F:459:ALA:N	2.68	0.51
2:B:452:LYS:HG2	2:B:456:ARG:NE	2.15	0.51
2:F:459:ALA:HA	2:F:468:GLU:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:402:NAG:O6	4:C:502:HOH:O	2.18	0.51
1:E:95:LEU:HA	1:E:230:TYR:HB2	1.93	0.50
2:B:452:LYS:CG	2:B:456:ARG:HE	2.14	0.50
2:D:458:ASN:HB3	2:D:471:HIS:HE1	1.71	0.50
1:C:202:MET:HE2	1:C:243:VAL:HG13	1.94	0.50
1:E:18:THR:HB	2:F:434:GLU:HG3	1.94	0.50
1:A:290:THR:HB	1:A:292:LYS:H	1.77	0.50
1:C:304:GLU:OE1	2:D:391:GLN:NE2	2.45	0.50
2:D:379:ASN:OD1	1:E:22:LYS:HD2	2.12	0.50
1:E:129:ARG:NH1	1:E:155:ASP:OD2	2.42	0.50
2:F:333:GLY:O	2:F:337:GLY:HA3	2.12	0.50
2:D:371:GLN:HB2	2:D:374:ILE:HB	1.92	0.50
1:E:2:LYS:HG2	2:F:468:GLU:HA	1.93	0.50
2:D:357:ASN:HD21	2:D:475:ASN:ND2	2.10	0.50
2:F:450:LYS:O	2:F:454:GLN:HG2	2.12	0.50
1:C:263:LYS:C	1:C:264:LYS:CG	2.85	0.49
2:B:434:GLU:OE1	2:F:435:ARG:NH1	2.44	0.49
2:B:461:ASP:HB2	2:B:467:PHE:CE2	2.48	0.49
2:D:355:HIS:O	2:D:361:SER:OG	2.12	0.49
2:F:455:LEU:HD23	2:F:486:TYR:CD2	2.47	0.49
2:B:470:TRP:CE2	2:B:471:HIS:HB2	2.47	0.49
2:F:462:LEU:HD12	2:F:468:GLU:CD	2.37	0.49
1:C:5:ILE:HD13	2:D:467:PHE:HE1	1.78	0.49
1:E:210:ALA:C	1:E:211:LYS:HG2	2.38	0.49
2:D:462:LEU:HD11	2:D:468:GLU:HB2	1.94	0.49
2:B:458:ASN:C	2:B:470:TRP:HB2	2.38	0.49
1:C:81:GLU:O	1:C:269:LYS:HA	2.13	0.48
2:F:457:ASP:C	2:F:459:ALA:H	2.19	0.48
1:C:127:THR:HG22	1:C:151:LEU:HD22	1.93	0.48
1:C:18:THR:HB	2:D:434:GLU:HG3	1.93	0.48
1:E:262:ASN:H	1:E:263:LYS:HD2	1.77	0.48
1:E:289:LYS:HG3	1:E:289:LYS:O	2.12	0.48
2:F:460:ASN:ND2	2:F:461:ASP:N	2.61	0.48
2:D:371:GLN:HA	2:D:374:ILE:H	1.77	0.48
2:B:479:GLU:O	2:B:483:ASN:HB2	2.14	0.48
1:E:119:LYS:HD3	1:E:127:THR:HB	1.96	0.48
2:B:480:SER:HB2	2:B:486:TYR:HB2	1.96	0.48
1:A:95:LEU:HA	1:A:230:TYR:HB2	1.95	0.47
1:E:91:TYR:HD2	1:E:132:THR:HG21	1.79	0.47
1:C:2:LYS:HZ3	2:D:466:CYS:CB	2.27	0.47
1:E:1:ASP:O	1:E:2:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD2	1:A:271:ASP:N	2.41	0.47
1:A:293:THR:HG23	1:A:294:PHE:CD2	2.49	0.47
1:C:263:LYS:C	1:C:264:LYS:HG2	2.39	0.47
2:F:469:PHE:HE1	2:F:472:LYS:C	2.23	0.47
2:B:340:GLU:H	2:B:340:GLU:HG2	1.52	0.47
1:E:236:ARG:HG3	1:E:239:GLU:CD	2.40	0.47
1:E:2:LYS:HD2	2:F:469:PHE:N	2.30	0.47
2:F:332:PHE:CE1	2:F:442:ALA:HB2	2.51	0.46
2:D:472:LYS:HE3	2:D:472:LYS:HB3	1.70	0.46
2:F:461:ASP:HA	2:F:468:GLU:OE1	2.15	0.46
2:B:458:ASN:OD1	2:B:488:TYR:CE1	2.69	0.46
2:D:357:ASN:ND2	2:D:359:GLN:OE1	2.49	0.46
1:A:91:TYR:HD2	1:A:132:THR:HG21	1.81	0.46
1:A:53:LYS:HA	1:A:53:LYS:HD3	1.80	0.46
1:A:210:ALA:C	1:A:211:LYS:HG2	2.41	0.46
2:B:348:ASP:OD2	2:B:365:ALA:N	2.48	0.46
1:C:200:VAL:HG13	1:C:249:LEU:HD13	1.98	0.46
2:F:338:PHE:CE1	2:F:339:ILE:HG13	2.50	0.46
1:E:2:LYS:HD3	2:F:469:PHE:CD2	2.45	0.46
2:F:432:GLU:OE1	2:F:435:ARG:NH2	2.38	0.46
2:F:457:ASP:O	2:F:470:TRP:CD1	2.69	0.46
2:F:469:PHE:HD1	2:F:471:HIS:NE2	2.14	0.46
1:A:214:GLU:CD	1:E:210:ALA:HB3	2.41	0.45
2:D:479:GLU:O	2:D:483:ASN:HB2	2.17	0.45
1:E:261:THR:C	1:E:263:LYS:H	2.24	0.45
1:A:218:ARG:O	1:A:225:ARG:HG2	2.16	0.45
1:C:155:ASP:O	1:C:156:SER:HB3	2.16	0.45
1:E:129:ARG:O	1:E:129:ARG:CG	2.63	0.45
1:C:34:GLU:OE1	1:C:290:THR:OG1	2.34	0.45
2:D:392:PHE:HZ	2:D:413:MET:HE3	1.82	0.45
2:D:478:MET:O	2:D:481:VAL:HG22	2.17	0.45
2:B:458:ASN:O	2:B:470:TRP:HB2	2.16	0.45
2:B:453:SER:O	2:B:453:SER:OG	2.35	0.45
2:B:376:GLY:HA2	1:C:20:LEU:O	2.17	0.45
2:D:376:GLY:O	2:D:379:ASN:HB3	2.16	0.44
1:A:202:MET:HE2	1:A:243:VAL:HG13	1.99	0.44
1:E:1:ASP:HB3	2:F:469:PHE:CE2	2.51	0.44
1:C:209:PHE:CZ	1:C:211:LYS:HG3	2.53	0.44
2:D:487:ASP:OD1	2:D:487:ASP:N	2.51	0.44
1:E:41:PHE:CE2	1:E:272:LEU:HB2	2.52	0.44
2:F:416:GLY:O	2:F:420:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:GLY:O	2:B:420:VAL:HG13	2.17	0.44
2:B:461:ASP:HB2	2:B:467:PHE:HE2	1.81	0.44
2:D:485:THR:HG21	3:D:501:NAG:H82	1.98	0.44
1:C:325:GLN:HE22	2:D:342:GLY:C	2.14	0.44
1:E:263:LYS:HD2	1:E:263:LYS:N	2.30	0.44
1:C:91:TYR:OH	1:C:224:GLN:NE2	2.51	0.44
2:F:475:ASN:HA	2:F:478:MET:HB2	2.00	0.44
1:A:10:ASN:ND2	4:A:503:HOH:O	2.10	0.44
1:C:41:PHE:CE2	1:C:272:LEU:HB2	2.53	0.44
1:A:263:LYS:HE3	1:A:263:LYS:HB3	1.68	0.43
1:E:56:THR:HG22	1:E:85:ALA:HB3	2.00	0.43
1:A:309:VAL:CG2	2:B:422:THR:HA	2.49	0.43
1:E:202:MET:HE2	1:E:243:VAL:HG13	2.00	0.43
2:F:458:ASN:HD22	2:F:458:ASN:HA	1.64	0.43
1:C:325:GLN:NE2	2:D:342:GLY:N	2.67	0.43
2:D:371:GLN:CA	2:D:374:ILE:HB	2.49	0.43
1:E:46:ASN:C	1:E:47:LYS:HD3	2.44	0.43
1:C:2:LYS:HD2	1:C:3:ILE:N	2.34	0.43
1:C:53:LYS:HB3	1:C:53:LYS:HE3	1.63	0.43
1:C:107:SER:O	1:C:261:THR:HG22	2.19	0.43
1:C:288:LEU:HD21	1:C:297:VAL:HG21	2.00	0.43
2:B:413:MET:HB3	2:B:413:MET:HE2	1.77	0.43
1:C:119:LYS:HD3	1:C:127:THR:HB	2.01	0.43
2:F:413:MET:HE2	2:F:413:MET:HB3	1.87	0.43
2:D:459:ALA:HA	2:D:468:GLU:O	2.19	0.42
1:E:1:ASP:O	1:E:2:LYS:CB	2.66	0.42
1:E:156:SER:OG	1:E:157:ALA:N	2.48	0.42
1:C:8:HIS:ND1	2:D:349:GLY:O	2.52	0.42
1:E:81:GLU:O	1:E:269:LYS:HA	2.19	0.42
1:A:5:ILE:CD1	2:B:451:VAL:HG11	2.49	0.42
2:B:483:ASN:OD1	2:B:485:THR:OG1	2.36	0.42
2:D:413:MET:HB3	2:D:413:MET:HE2	1.75	0.42
1:E:263:LYS:HB3	1:E:264:LYS:CG	2.47	0.42
1:A:41:PHE:CE2	1:A:272:LEU:HB2	2.55	0.42
2:D:352:GLY:HA2	2:D:366:ASP:H	1.84	0.42
2:D:353:TYR:CD1	2:D:482:LYS:HE2	2.54	0.42
1:C:1:ASP:OD2	2:D:472:LYS:HB3	2.20	0.42
2:D:376:GLY:HA2	1:E:20:LEU:O	2.20	0.42
1:E:262:ASN:HB3	1:E:263:LYS:HD2	2.02	0.42
1:E:307:LYS:HE3	2:F:390:THR:O	2.19	0.42
1:A:8:HIS:O	1:A:320:LEU:HD11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:N	2:B:348:ASP:OD1	2.53	0.42
1:E:302:ILE:HD12	1:E:302:ILE:HA	1.96	0.42
2:D:359:GLN:NE2	2:D:474:ASP:HA	2.35	0.42
1:E:2:LYS:CG	2:F:469:PHE:H	2.33	0.42
1:A:32:LEU:HB3	1:A:293:THR:CG2	2.50	0.41
1:C:65:PRO:HG3	1:C:144:PHE:O	2.19	0.41
1:C:37:LYS:HD3	1:C:297:VAL:HG13	2.02	0.41
1:E:182:HIS:CE1	1:E:214:GLU:HG3	2.55	0.41
2:B:338:PHE:CE1	2:B:339:ILE:HG13	2.55	0.41
1:E:135:CYS:O	1:E:143:SER:HB3	2.20	0.41
1:A:5:ILE:HD11	2:B:451:VAL:HG11	2.02	0.41
1:A:58:GLU:OE2	4:A:504:HOH:O	2.22	0.41
1:E:133:ASN:HA	1:E:141:ASP:O	2.20	0.41
1:E:213:PRO:HG3	1:E:248:ASN:CG	2.46	0.41
2:F:474:ASP:OD1	2:F:474:ASP:C	2.62	0.41
1:C:8:HIS:O	1:C:320:LEU:HD11	2.21	0.41
1:E:65:PRO:HG3	1:E:144:PHE:O	2.20	0.41
1:E:149:VAL:HG13	1:E:251:ALA:HB3	2.02	0.41
2:F:486:TYR:CD1	2:F:487:ASP:N	2.89	0.41
2:D:355:HIS:CE1	2:D:361:SER:HA	2.56	0.41
2:D:458:ASN:O	2:D:469:PHE:HA	2.21	0.41
1:E:201:ARG:HG2	1:E:210:ALA:CB	2.51	0.41
2:F:451:VAL:HG22	2:F:467:PHE:CZ	2.56	0.41
1:C:41:PHE:HB2	1:C:274:ILE:HG12	2.03	0.40
1:A:288:LEU:HD21	1:A:297:VAL:HG21	2.02	0.40
2:D:354:HIS:CE1	2:D:361:SER:OG	2.75	0.40
2:F:335:ILE:N	2:F:441:ASP:OD1	2.50	0.40
2:F:367:ARG:HA	2:F:367:ARG:HD2	1.76	0.40
2:B:464:ASN:OD1	2:B:464:ASN:C	2.65	0.40
2:F:463:GLY:C	2:F:465:GLY:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/325 (99%)	306 (95%)	15 (5%)	2 (1%)	21	42
1	C	323/325 (99%)	306 (95%)	13 (4%)	4 (1%)	10	23
1	E	323/325 (99%)	308 (95%)	12 (4%)	3 (1%)	14	30
2	B	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	6	13
2	D	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	9	21
2	F	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	21	42
All	All	1440/1452 (99%)	1365 (95%)	60 (4%)	15 (1%)	12	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
2	B	480	SER
1	C	156	SER
1	C	263	LYS
2	D	483	ASN
1	E	264	LYS
2	B	474	ASP
1	C	155	ASP
1	E	2	LYS
1	E	156	SER
2	F	474	ASP
1	A	156	SER
2	B	470	TRP
2	D	474	ASP
1	C	262	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/285 (100%)	277 (97%)	8 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/285 (100%)	278 (98%)	7 (2%)	42	69
1	E	285/285 (100%)	275 (96%)	10 (4%)	32	59
2	B	134/134 (100%)	128 (96%)	6 (4%)	24	50
2	D	134/134 (100%)	124 (92%)	10 (8%)	12	28
2	F	134/134 (100%)	121 (90%)	13 (10%)	8	17
All	All	1257/1257 (100%)	1203 (96%)	54 (4%)	26	51

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	95	LEU
1	A	121	THR
1	A	155	ASP
1	A	156	SER
1	A	263	LYS
1	A	289	LYS
1	A	290	THR
2	B	340	GLU
2	B	348	ASP
2	B	368	GLU
2	B	434	GLU
2	B	451	VAL
2	B	470	TRP
1	C	2	LYS
1	C	14	THR
1	C	86	GLN
1	C	163	LYS
1	C	264	LYS
1	C	290	THR
1	C	309	VAL
2	D	344	THR
2	D	358	SER
2	D	368	GLU
2	D	370	THR
2	D	371	GLN
2	D	396	ASP
2	D	445	LYS
2	D	454	GLN
2	D	481	VAL

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Mol	Chain	Res	Type
2	D	487	ASP
1	E	2	LYS
1	E	37	LYS
1	E	53	LYS
1	E	95	LEU
1	E	140	LEU
1	E	262	ASN
1	E	264	LYS
1	E	269	LYS
1	E	277	CYS
1	E	320	LEU
2	F	347	ILE
2	F	358	SER
2	F	367	ARG
2	F	368	GLU
2	F	434	GLU
2	F	451	VAL
2	F	454	GLN
2	F	458	ASN
2	F	460	ASN
2	F	461	ASP
2	F	469	PHE
2	F	472	LYS
2	F	483	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	172	GLN
1	A	224	GLN
2	B	357	ASN
2	B	397	HIS
2	B	454	GLN
2	B	471	HIS
1	C	172	GLN
1	C	224	GLN
2	D	355	HIS
2	D	454	GLN
2	D	458	ASN
2	D	475	ASN
1	E	87	ASN

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Mol	Chain	Res	Type
1	E	96	ASN
1	E	262	ASN
2	F	458	ASN
2	F	460	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	402	1	14,14,15	0.24	0	17,19,21	0.62	1 (5%)
3	NAG	E	402	1	14,14,15	0.23	0	17,19,21	0.81	1 (5%)
3	NAG	D	501	2	14,14,15	0.63	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	C	401	1	14,14,15	0.54	0	17,19,21	0.60	0
3	NAG	E	401	1	14,14,15	1.35	2 (14%)	17,19,21	1.03	1 (5%)
3	NAG	A	401	1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
3	NAG	C	402	1	14,14,15	0.31	0	17,19,21	0.90	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	2/6/23/26	0/1/1/1
3	NAG	D	501	2	-	2/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	C	402	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	NAG	C1-C2	3.86	1.57	1.52
3	E	401	NAG	O5-C1	2.91	1.48	1.43
3	D	501	NAG	C1-C2	2.04	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAG	C1-O5-C5	2.93	116.11	112.19
3	D	501	NAG	C1-O5-C5	-2.69	108.58	112.19
3	E	402	NAG	C1-O5-C5	2.56	115.61	112.19
3	A	401	NAG	C1-O5-C5	2.31	115.28	112.19
3	E	401	NAG	O3-C3-C4	2.24	115.66	110.38
3	A	402	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
3	D	501	NAG	O5-C5-C6-O6
3	D	501	NAG	C4-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	401	NAG	C4-C5-C6-O6
3	E	402	NAG	O5-C5-C6-O6
3	C	402	NAG	O5-C5-C6-O6
3	E	402	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	NAG	3	0
3	C	402	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	325/325 (100%)	0.36	13 (4%)	42 37	32, 54, 92, 147	0
1	C	325/325 (100%)	0.49	12 (3%)	45 39	33, 57, 106, 154	0
1	E	325/325 (100%)	0.74	27 (8%)	17 13	39, 71, 110, 168	0
2	B	159/159 (100%)	1.04	28 (17%)	4 3	40, 85, 164, 215	0
2	D	159/159 (100%)	1.09	22 (13%)	6 5	37, 96, 166, 232	0
2	F	159/159 (100%)	1.03	24 (15%)	5 4	37, 95, 174, 220	0
All	All	1452/1452 (100%)	0.70	126 (8%)	16 12	32, 67, 146, 232	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	353	TYR	6.1
2	B	455	LEU	5.6
2	F	467	PHE	5.6
2	F	344	THR	5.2
1	E	138	TYR	5.1
1	A	157	ALA	4.9
2	D	455	LEU	4.9
2	D	467	PHE	4.5
2	B	470	TRP	4.5
2	B	488	TYR	4.3
2	D	396	ASP	3.9
2	D	445	LYS	3.9
2	B	469	PHE	3.8
2	F	469	PHE	3.8
1	A	141	ASP	3.7
1	E	157	ALA	3.7
1	E	2	LYS	3.4
2	D	360	GLY	3.4
1	E	139	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	330	GLY	3.3
2	D	470	TRP	3.2
2	D	461	ASP	3.2
2	D	463	GLY	3.1
1	E	325	GLN	3.1
1	C	324	PRO	3.1
2	F	455	LEU	3.1
1	A	158	THR	3.1
2	B	476	GLU	3.1
2	F	345	GLY	3.1
1	A	155	ASP	3.0
2	B	471	HIS	3.0
1	E	277	CYS	3.0
2	D	358	SER	3.0
2	F	451	VAL	2.9
2	F	463	GLY	2.9
2	B	442	ALA	2.9
1	C	321	ARG	2.8
1	E	185	ASP	2.8
2	B	458	ASN	2.7
2	B	481	VAL	2.7
2	F	331	ILE	2.7
2	D	488	TYR	2.7
1	C	157	ALA	2.7
1	E	5	ILE	2.7
2	D	472	LYS	2.7
2	B	451	VAL	2.7
2	B	468	GLU	2.7
1	A	140	LEU	2.6
1	E	210	ALA	2.6
1	E	271	ASP	2.6
1	E	158	THR	2.6
2	F	471	HIS	2.6
2	F	462	LEU	2.6
1	E	187	THR	2.6
1	E	265	GLY	2.5
1	E	69	LEU	2.5
1	E	4	CYS	2.5
2	F	459	ALA	2.5
2	D	344	THR	2.5
2	F	478	MET	2.5
1	A	5	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	470	TRP	2.5
2	B	467	PHE	2.5
2	F	483	ASN	2.5
1	A	277	CYS	2.5
2	D	351	TYR	2.5
1	E	3	ILE	2.5
2	F	460	ASN	2.5
1	A	156	SER	2.5
2	D	355	HIS	2.5
1	A	3	ILE	2.4
2	B	487	ASP	2.4
1	C	140	LEU	2.4
1	E	140	LEU	2.4
2	F	332	PHE	2.4
1	E	309	VAL	2.4
2	F	488	TYR	2.4
1	E	264	LYS	2.4
1	C	154	THR	2.3
2	B	478	MET	2.3
1	A	138	TYR	2.3
1	A	37	LYS	2.3
2	F	334	ALA	2.3
1	E	215	ILE	2.3
2	B	359	GLN	2.3
2	D	352	GLY	2.3
2	F	359	GLN	2.3
2	D	331	ILE	2.3
2	D	465	GLY	2.3
1	C	20	LEU	2.3
1	E	300	LEU	2.3
2	F	481	VAL	2.3
2	B	364	ALA	2.2
2	D	462	LEU	2.2
2	F	358	SER	2.2
1	A	84	ASN	2.2
2	B	473	CYS	2.2
1	C	6	GLY	2.2
2	B	484	GLY	2.2
1	E	278	ASP	2.2
1	C	261	THR	2.2
2	B	486	TYR	2.2
1	A	320	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	45	MET	2.2
1	C	3	ILE	2.2
2	F	367	ARG	2.2
1	E	85	ALA	2.1
2	B	459	ALA	2.1
2	F	484	GLY	2.1
1	C	217	ALA	2.1
2	D	341	GLY	2.1
1	C	158	THR	2.1
1	C	45	MET	2.1
2	B	485	THR	2.1
1	E	1	ASP	2.1
2	B	351	TYR	2.1
2	D	448	TYR	2.1
2	B	477	CYS	2.1
2	B	456	ARG	2.0
1	E	84	ASN	2.0
2	F	468	GLU	2.0
1	E	323	VAL	2.0
2	D	332	PHE	2.0
2	D	469	PHE	2.0
2	B	475	ASN	2.0
2	B	354	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	401	14/15	0.43	0.15	119,124,128,129	0
3	NAG	D	501	14/15	0.49	0.17	166,171,173,174	0
3	NAG	C	401	14/15	0.52	0.18	140,159,164,164	0
3	NAG	E	402	14/15	0.75	0.11	64,80,88,88	0
3	NAG	E	401	14/15	0.76	0.13	140,148,152,154	0
3	NAG	C	402	14/15	0.78	0.15	78,93,104,107	0
3	NAG	A	402	14/15	0.78	0.13	66,80,93,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.